

Pfizer: NMR to ADF

Bo Du

Justin Van Duine



WORLDWIDE RESEARCH & DEVELOPMENT
Medicinal Sciences

Together, let's get it right the first time.

Pfizer Data: Scientific Data Cloud (SDC)

Capture



Lab Instruments & Software



Manufacturing Equipment



Lab IT Systems

Use



Mobile Devices



Reports



Data automatically swept into the cloud

Data is made available to systems and reports

IDF
Scientific Data Cloud

Predict

Provides data need to build/run models

Predicted output from models is stored



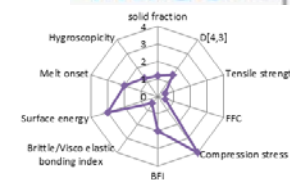
Computational Models



Hosting Platforms

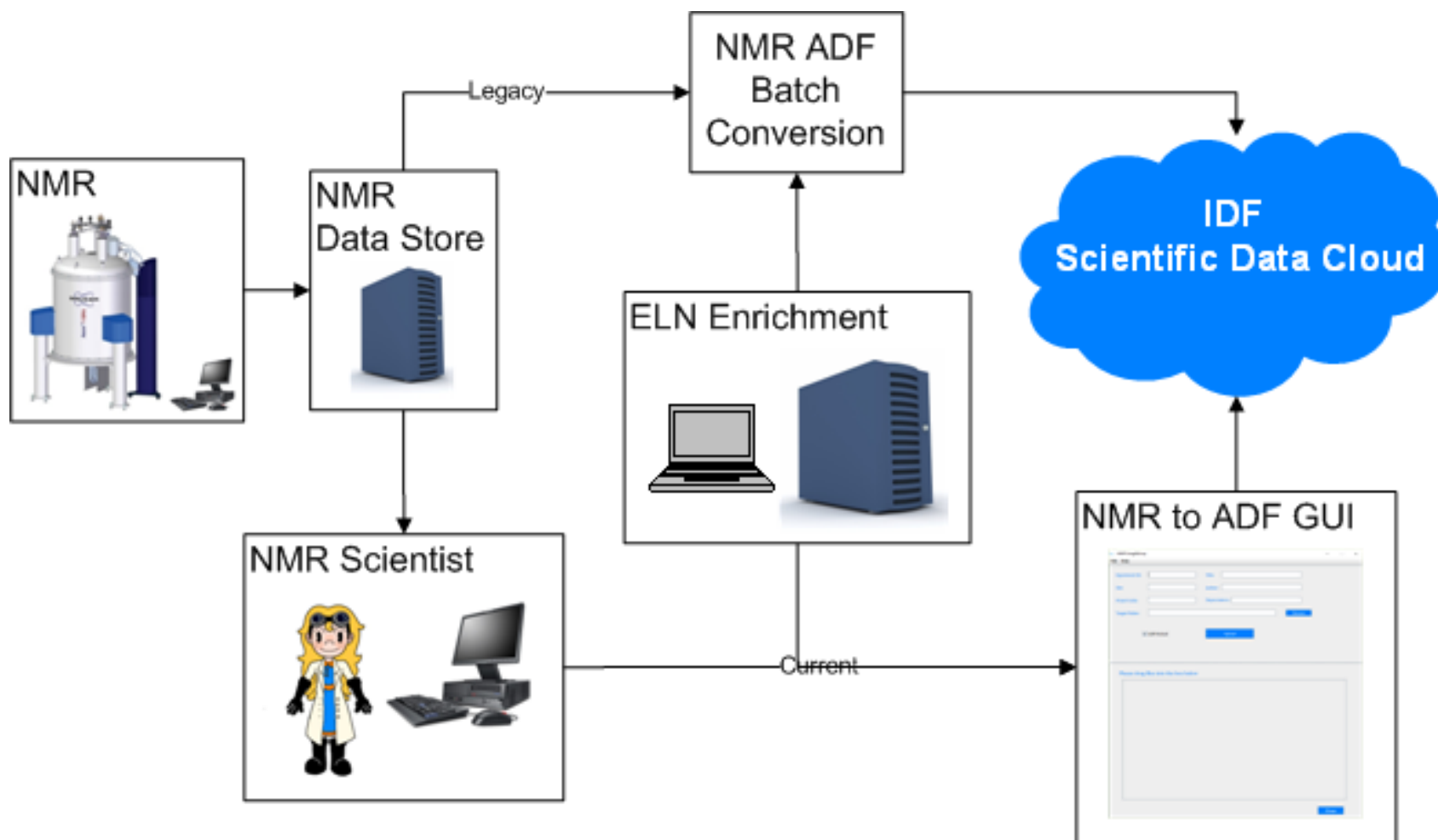
Visualization tools are configured to pull data from the cloud

Reuse



Data Visualization

Pfizer: NMR to ADF Process Flow



Enhancements to the Boehringer NMR Converter

- Transformed the user interface from a command line into a Graphic User Interface (GUI)
 - Encourages user adoption
 - Batch processing version is also available
- Uses current released versions of the Allotrope API's
- Extended to include 3D NMR data
- Added “Peak Table” to the Data Cube
- Creates a “Companion” JSON file to facilitate searching in the Pfizer SDC
- Added “important” meta data (including that from Pfizer's ELN) to the Data Description as literals
 - Does not use BFO/ADM



NMR to ADF Functionality (Converter GUI)

NMR Drag&Drop

File Help

Experiment ID: Title:

Site: Author:

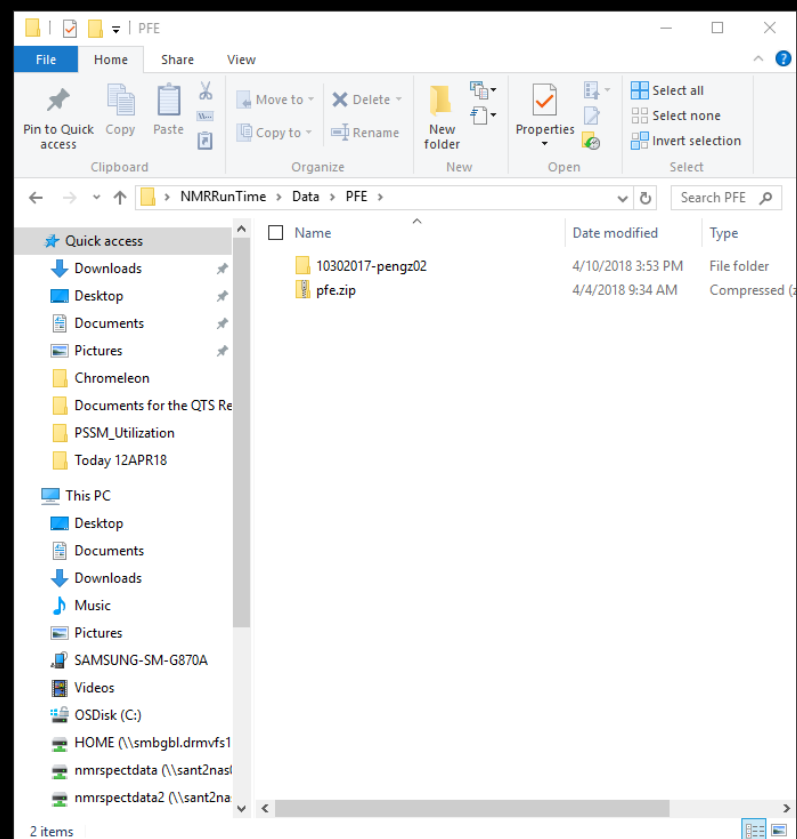
Project Code: Department:

Target Folder:

☒ ADF Format

Please drag files into the box below

Taskbar: E3project Pic New folder Biovia View_Detai... Record a IDF Konnect SQLDevelo... The-allotro... WebEx Me...



NMR to ADF Functionality

The image displays the NMR Drag&Drop application interface and a Windows File Explorer window illustrating the drag-and-drop functionality.

NMR Drag&Drop Application Interface:

- Form Fields:**
 - Experiment ID: 00705863-0923
 - Title: fluorobutanesulfonyl fluoride (NFF)
 - Site: USA - CT -
 - Author: Peng, Zhihui
 - Project Code: 7PB792B000
 - Department: PSSM Chemical R&D
 - Target Folder: (empty)
- Buttons:** Upload, Browse, Clear
- Checkboxes:** ☒ ADF Format
- File List:**
 - C:\Users\vanduij\Desktop\NMRRunTime\Data\PFE\10302017-pengz021
 - C:\Users\vanduij\Desktop\NMRRunTime\Data\PFE\10302017-pengz022
 - C:\Users\vanduij\Desktop\NMRRunTime\Data\publicexam1d_1Dsf1
 - 2D C:\Users\vanduij\Desktop\NMRRunTime\Data\publicexam2d_2Dsf13
 - 3D C:\Users\vanduij\Desktop\NMRRunTime\Data\publicexam3d_3Dsf1

Windows File Explorer (PFE):

- Path:** NMRRunTime > Data > PFE
- Files:** 10302017-pengz02, pfe.zip

Annotations:

- ELN Enrichment:** A red box highlights the form fields.
- Autodetect 1, 2 and 3D NMR Experiments:** A red box highlights the file list.
- Drag & Drop:** A red oval and arrow indicate the action of dragging files from the File Explorer to the application interface.



NMR to ADF Functionality

The image displays two windows illustrating the NMR to ADF functionality. On the left is the 'NMR Drag&Drop' application window, and on the right is a Windows File Explorer window showing the 'ADF Output' folder.

NMR Drag&Drop Application:

- Experiment ID:** 00705863-0923
- Title:** fluorobutanesulfonyl fluoride (NFF)
- Site:** USA - CT -
- Author:** Peng, Zhihui
- Project Code:** 7PB792B000
- Department:** PSSM Chemical R&D
- Target Folder:** C:\Users\vanduij\Desktop\NMRRunTime\ADF Output
- ☒ ADF Format
- Upload** button
- Drag-and-drop area with text: "Please drag files into the box below"
- Clear** button

ADF Output Folder (File Explorer):

Name	Date modified	Type
10302017-pengz02_1_1D-04-16-2018.adf	4/16/2018 1:21 PM	ADF
10302017-pengz02_1_1D-04-16-2018.adf.json	4/16/2018 1:21 PM	JSON
10302017-pengz02_2_1D-04-16-2018.adf	4/16/2018 1:21 PM	ADF
10302017-pengz02_2_1D-04-16-2018.adf.json	4/16/2018 1:21 PM	JSON

Red annotations highlight the workflow: an oval labeled 'Upload' points to the 'Upload' button in the application, and another oval labeled 'ADF on the SDC' points to the files in the 'ADF Output' folder.

Companion File (JSON)

ELN Enriched Metadata

```
{ "adfFilename": "C:\\Users\\vanduij\\Desktop\\NMRRunTime\\ADF
Output/10302017-pengz02_1_1D-04-16-2018.adf", "expID": "01234567-
0089", "title": "ABCD3: Telescope acetone formation of PF-43210123 and
fluorination with perfluorobutanesulfonyl fluoride (NfF)", "site": "USA -
CT -", "author": "Peng, Zhihui", "projCode": "7PB792B000", "department": "PSSM
Chemical
R\\u0026D", "nmrType": "1d", "rawFolder": "C:\\Users\\vanduij\\Desktop\\NMRRun
Time\\Data\\PFE\\10302017-pengz02\\1", "filename": "10302017-pengz02_1_1D-
04-16-2018.adf", "PFnum": "PF-43210123", "keyword": "Reaction
Development", "firstName": "John", "lastName": "Doe", "benchtopOperator": "VAND
UIJ", "benchtopComputerName": "CMRLXX00CYYS", "fileCreated": "2018.04.16
13:21:19", "guid": "a2a380d5-c7db-455f-b4f7-
c67392a2b48d", "fileLength": 3852316, "md5": "881289f6a1e42dc11f4df7161ba346a
```

```
SubcubeMask": [3,0,0,0,0,0,0,0], "FIDDataType": "I4", "SPCDataType": "I4
", "NominalFIDPoints": [32768,0,0,0,0,0,0,0], "NominalSPCPoints": [65536,0,0,
0,0,0,0,0], "numScans": 16, "numDummyScans": 2, "InitDigitizerResolution": 22, "
FinalDigitizerResolutions": -
999, "PowerLevel": 120, "AcqMode": 3, "DecimationDigitalFilter": 2496, "DSPFirmw
areVersion": 20, "title": "705863-923crude#1PROTON CDCl3
{C:\\opt\\topspin3.2} Doe 11
", "AcqDate": "30-Oct-
17", "AcqSWName": "TopSpin", "AcqSWVersion": "", "solvent": "CDCl3", "PulseProg"
: "zg30", "AutoProg": "au_zg", "GradientProg": "", "CompPulseDecouplingProg": ""
, "DecouplerPower": "", "ObsNucleus": "1H", "fileExt": "", "origDataPath": "C:\\U
sers\\vanduij\\Desktop\\NMRRunTime\\Data\\PFE\\
\\u0000\\u0000\\u0000\\u0000\\u0000\\u0000\\u0000\\u0000\\u0000\\u0000\\u0000"
```

NMR Literal Metadata

ADF Explorer

[illegible]